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Sustainable Catalytic CO_2 Conversion to Value-Added Chemicals: From Catalyst Design to Device Development

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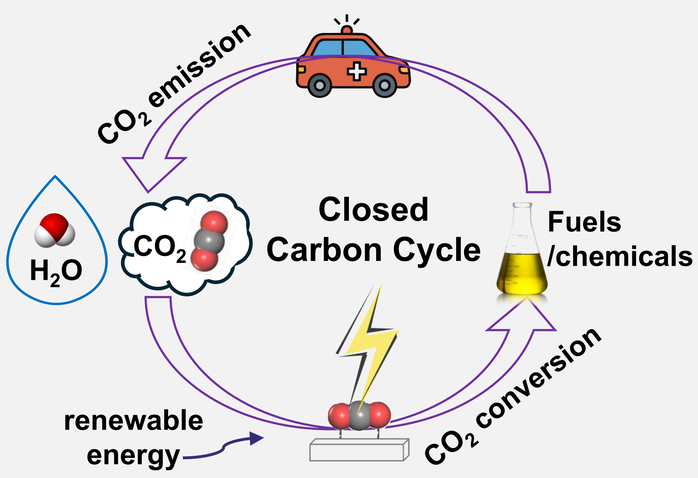
Introduction

Background



Motivation

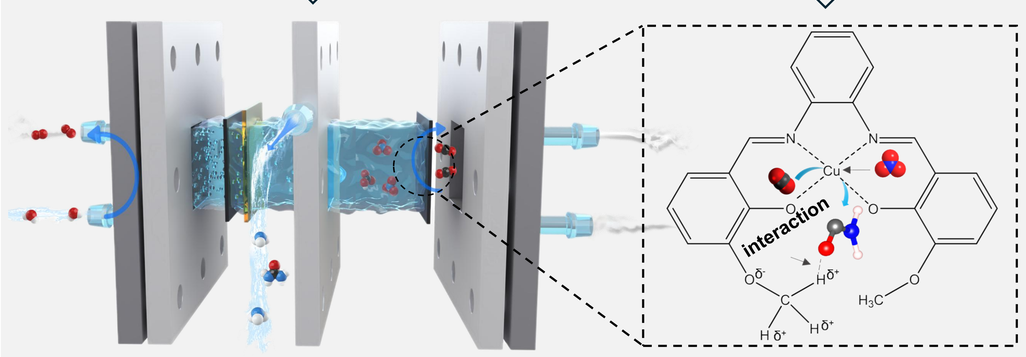
- To convert exiting CO_2 emissions back to valuable chemicals
- To reduce high CO_2 emissions during industrial manufacturing of urea
- To transform chemical industrial manufacturing in a sustainable way

Challenge

- Unclear mechanism during reactions
- Low efficiency of catalysts
- Low production rate in reactors

Methodology

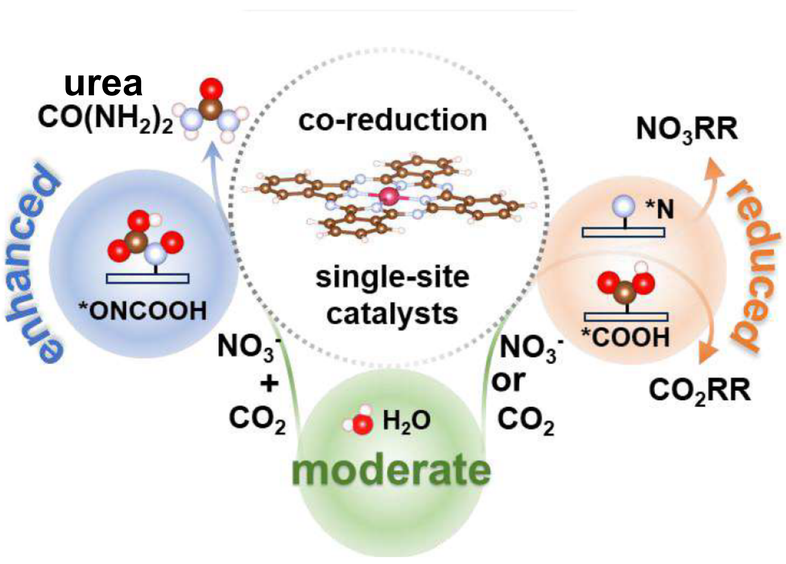
Sustainable catalytic CO_2 conversion based on device development[1-3] + catalyst design[4-6]

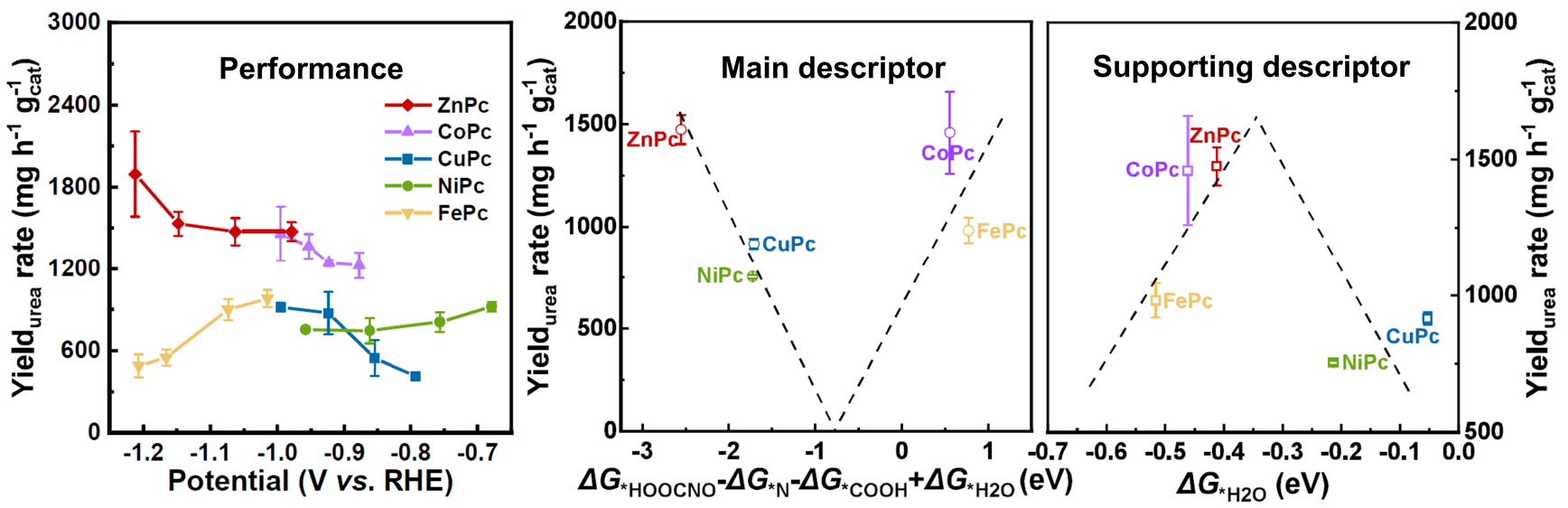


Key Findings

1. Mechanistic Exploration

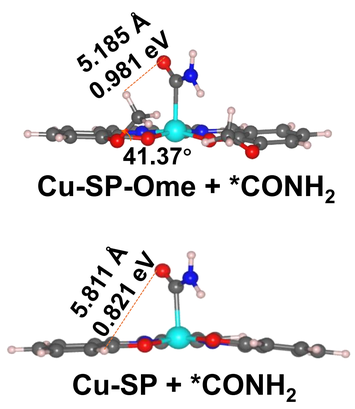
➢ $\Delta G_{*HOOCNO}-\Delta G_{*N}-\Delta G_{*COOH}+\Delta G_{*H2O}$ can be a potential descriptor for urea formation.[5]

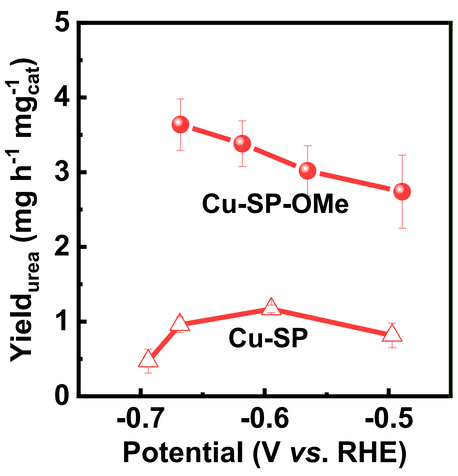




2. Catalyst Design

Optimized binding ⇨ **Increased yields on catalysts**

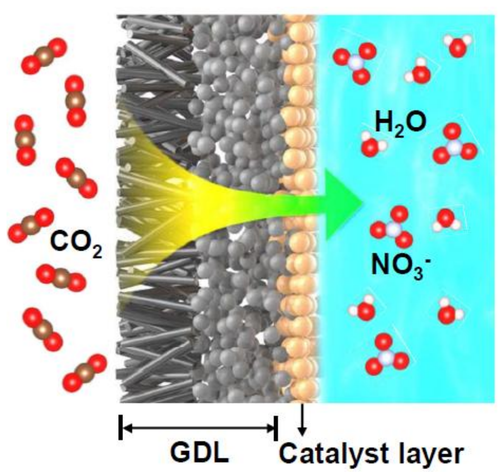


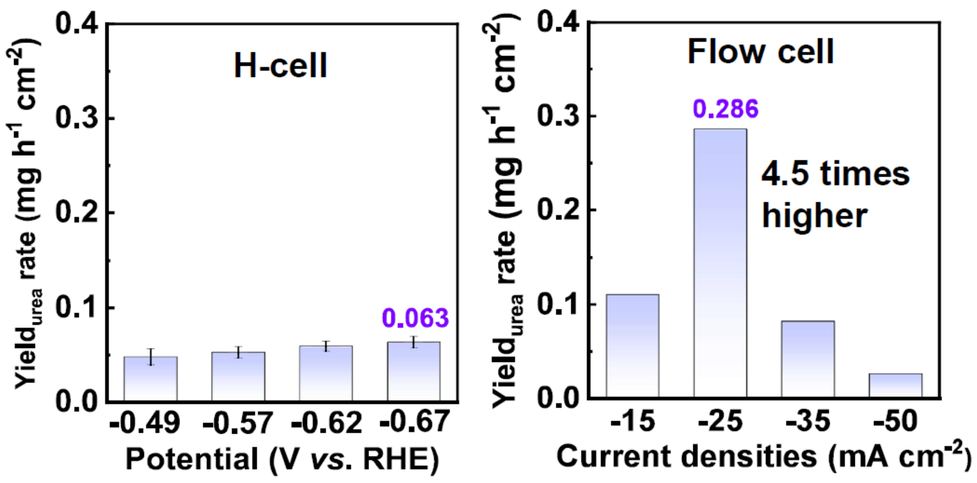


➢ The substituted $-OCH_3$ group helps binding *$CONH_2$ during C-N coupling process toward urea formation.[2]

3. Device Development

Three-phase interface engineering ⇨ **Improved production in flow cell**





➢ The creation of gas-solid-liquid three-phase interface[1] eliminates mass transport issue caused by low solubility of CO_2,[2] promoting reaction process.

Summary and Perspectives

- CO_2-involved electrocatalytic conversion offers a highly **sustainable pathway** for producing value-added chemicals using renewable electricity.
- **High-activity and high-selectivity catalysts** are the key to achieving high-performance conversion to desired products.
- **Device development** is critical for overcoming mass transport limitations at reaction interface and achieving industrially relevant production rates.
- Descriptors can be integrated with **artificial intelligence** to guide rational design and accelerate screening of potential catalysts.

References

[1] Q. Zhao, et al., *Energy Environ. Sci.*, 2021,14, 5444.
[2] Q. Zhao, et al., *Angew. Chem. Int. Ed.* 2023, 62, e202307123.
[3] Q. Zhao, et al., *Nat Water*, 2026, under review.
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[6] Q. Zhao, et al., *Angew. Chem. Int. Ed.*, 2024, 63, e202314384.

Acknowledgements

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